TILDA-V: a full-differential Monte Carlo for describing the energy deposition at the nanometer scale for protons in biological matter

M. A. Quinto* [1], J. M. Monti*, P. F. Weck‡, O. A. Fojón*, R. D. Rivarola* and C. Champion†

*Instituto de Física Rosario, CONICET and Universidad Nacional de Rosario, Rosario, Argentina
‡Sandia National Laboratories, Albuquerque, NM 87185, USA
†Université de Bordeaux, CNRS/IN2P3, Centre d'Etudes Nucléaires de Bordeaux Gradignan, Gradignan

Synopsis The present study aims at scrutinizing at the nanometer scale the energy deposition of protons in a realistic biological medium. In this context, a self-consistent quantum mechanical modeling of the ionization and the electron capture processes is reported within the continuum distorted wave-eikonal initial state framework for both isolated water molecules and DNA components impacted by protons.

In the context of biomolecular radiation damage, primary charged particles loose energy during interaction with biological tissues, potentially leading to the creation of secondary electrons in the medium. Modeling the radiobiological damages induced by such ionizing particles crossing the living matter requires a precise knowledge of the full radiation history, including the energy deposited during inelastic collisions as well as the kinetic energy transferred to secondary particles eventually emitted. Monte-Carlo methods are among the best-suited tools to achieve that goal since they provide an adequate description of the radio-induced energetic pattern at the finest scale, *i.e.* at the cellular or sub-cellular level. However, the reliability of such numerical methods heavily depends on the accuracy of the input data used in the simulations, namely, the interaction cross sections needed for describing the various collisional processes involved in the slowing-down of the charged particles in the medium of interest [1].

The current work aims at scrutinizing the appropriateness of water vapor as a surrogate for modeling the main ionizing proton-induced processes in human tissue and revealing new insights into proton-induced energy transfers in realistic biological at the nano scale.

Figure 1 exhibits the energy deposition induced by protons in cylindrical volumes mimicking biological volumes of interest, namely, a 2-nm-diameter by 2-nm-length DNA-segment (upper panel) as well as a 10-nm-diameter by 5-nm-length nucleosome (lower panel). To investigate the role played by the biological medium description, the cylinders are successively filled by liquid water (1 g.cm^{-3}) and hydrated DNA (1.29 g.cm^{-3}) [1].

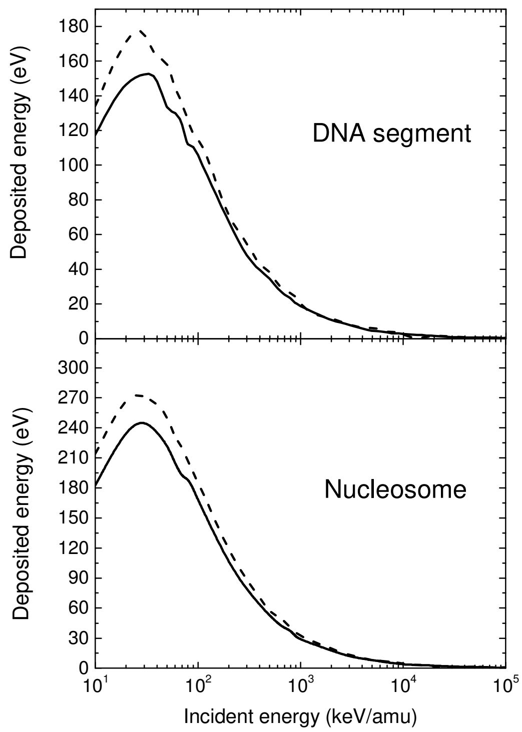

Figure 1. Energy deposition inside cylindrical volumes of biological interest: DNA segment (upper panel) and nucleosome (lower panel) successively filled with liquid water (solid line) and hydrated DNA (dashed line).

References

[1] C. Champion *et al.* 2015 *Phys. Med. Biol.* **60** 7805 - 7828

[1] E-mail: quinto@ifir-conicet.gov.ar